Spin-orbit splitting and the tensor component of the Skyrme interaction

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Abstract

We study the role of the tensor term of the Skyrme effective interactions on the spin-orbit splittings in the N=82 isotones and Z=50 isotopes. The different role of the triplet-even and triplet-odd tensor forces is pointed out by analyzing the spin-orbit splittings in these nuclei. The experimental isospin dependence of these splittings cannot be described by Hartree-Fock calculations employing the usual Skyrme parametrizations, but is very well accounted for when the tensor interaction is introduced. The capability of the Skyrme forces to reproduce binding energies and charge radii in heavy nuclei is not destroyed by the introduction of the tensor term. Finally, we also discuss the effect of the tensor force on the centroid of the Gamow-Teller states.

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Nuclei far from the stability valley open a new test ground for nuclear models. Recently, many experimental and theoretical efforts have been paid to study the structure and the reaction mechanisms in the nuclei near the drip lines. Modern radioactive nuclear beam facilities and experimental detector setups have revealed several unexpected effects in nuclei, such as the existence of haloes and skins [1], the modifications of shell closures [2] and the pygmy dipole resonances [3, 4].

One of the current topics is the role of the tensor interactions on the shell evolution of nuclei far from the stability line. The role of the tensor interactions in the evolution of the single-particle states was first discussed within the Skyrme Hartree-Fock (HF) framework by Fl. Stancu *et al.*, almost thirty years ago [5]. However, serious attempts have never been devoted, until very recently, to the study of its effects on the evolution of the shell structure in heavy exotic nuclei. In fact, the Skyrme parameter sets which are widely used in nuclear structure calculations do not include the tensor contribution. This contribution was included only in the so-called Skyrme-Landau parametrizations of Ref. [6].

In the present paper, we discuss the isospin dependence of the shell structure (in particular, the spin-orbit splitting) of the Z=50 isotopes and N=82 isotones. We use the HF plus Bardeen-Cooper-Schrieffer (BCS) approach, by employing a Skyrme parameter set plus the triplet-even and triplet-odd tensor zero-range tensor terms, which read

$$\begin{aligned} v_T \;=\; & \frac{T}{2}\{[(\sigma_1\cdot k')(\sigma_2\cdot k') - \frac{1}{3}(\sigma_1\cdot\sigma_2)k'^2]\delta(r_1-r_2) \\ & + \;\delta(r_1-r_2)[(\sigma_1\cdot k)(\sigma_2\cdot k) - \frac{1}{3}(\sigma_1\cdot\sigma_2)k^2]\} \\ & + \;U\{(\sigma_1\cdot k')\delta(r_1-r_2)(\sigma_1\cdot k) - \frac{1}{3}(\sigma_1\cdot\sigma_2)[k'\cdot\delta(r_2-r_2)k]\}. \end{aligned} \tag{1}$$

In the above expression, the operator $k=(\nabla_1-\nabla_2)/2i$ acts on the right and $k'=-(\nabla_1-\nabla_2)/2i$ acts on the left. The coupling constants T and U denote the strength of the triplet-even and triplet-odd tensor interactions, respectively; we treat these coupling constants as free parameters in the following study. The tensor interactions (1) give contributions both to the binding energy and to the spin-orbit splitting, which are, respectively, quadratic and linear in the proton and neutron spin-orbit densities,

$$J_q(r) = \frac{1}{4\pi r^3}\sum_i v_i^2(2j_i+1)\left[j_i(j_i+1) - l_i(l_i+1) - \frac{3}{4}\right]R_i^2(r). \tag{2}$$

In this expression $q=0(1)$ labels neutrons (protons), while where $i=n,l,j$ runs over all states having the given q. The v_i^2 is the BCS occupation probability of each orbital and $R_i(r)$ is the radial part of the wavefunction. It should be noticed that the exchange part of the central Skyrme interaction gives the same kind of contributions to the total energy density and spin-orbit splitting. The central exchange and tensor contributions to the energy density H are

$$\Delta H = \frac{1}{2}\alpha(J_n^2+J_p^2) + \beta J_n J_p. \tag{3}$$

The spin-orbit potential is given by

$$U_{s.o.}^{(q)} = \frac{W_0}{2r}\left(2\frac{d\rho_q}{dr} + \frac{d\rho_{q'}}{dr}\right) + \left(\alpha\frac{J_q}{r} + \beta\frac{J_{q'}}{r}\right), \tag{4}$$

where the first term on the r.h.s comes from the Skyrme spin-orbit interaction whereas the second term includes both the central exchange and the tensor contributions, that is, $\alpha = \alpha_C + \alpha_T$ and $\beta = \beta_C + \beta_T$. The central exchange contributions are written in terms of the usual Skyrme parameters,

$$\begin{aligned} \alpha_C &= \frac{1}{8}(t_1 - t_2) - \frac{1}{8}(t_1 x_1 + t_2 x_2) \\ \beta_C &= -\frac{1}{8}(t_1 x_1 + t_2 x_2). \end{aligned} \tag{5}$$

Basic definitions of all quantities derived from the Skyrme parameters can be found in Refs. [7, 8]. The tensor contributions are expressed as

$$\begin{aligned} \alpha_T &= \frac{5}{12} U \\ \beta_T &= \frac{5}{24}(T + U). \end{aligned} \tag{6}$$

The central exchange contributions (5) have been neglected when fitting most of the Skyrme parameter sets, and when performing most of the previous HF calculations. In this work, we employ the SLy5 parameter set [8] which has been fitted with the same protocol of the more widely used SLy4 set and should consequently have similar quality. In the case of SLy5, the central exchange contributions are included in the fit and we take them into account here.

Except for the double-magic systems, we perform HF-BCS in order to take into account the pairing correlations. Our pairing force is a zero-range, density-dependent one, namely

$$V = V_0 \left(1 - \left(\frac{\varrho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)}{\varrho_0} \right)^{\gamma} \right) \cdot \delta(\vec{r}_1 - \vec{r}_2). \tag{7}$$

The parameters of this force (that is, V_0=680 MeV$\cdot$fm^3, γ=1 and ϱ_0=0.16 fm^{-3}) have been fixed along the Z=50 isotopic chain in connection with the SLy4 set in Ref. [9]. Therefore, we employ the same force here both for the neutron and the proton pairing interactions in the 50-82 shell, neglecting small readjustments which could be made to account for the Coulomb anti-pairing effect in the case of protons.

Before coming to a detailed analysis of our results, let us mention the important general features associated with the tensor and the central exchange contributions to the spin-orbit splitting. The first point concerns the A-dependence (or isospin dependence) of the the first and second terms in the r.h.s. of Eq. (4). Since the Skyrme spin-orbit contributuion (proportional to W_0) gives a value of the spin-orbit splitting which is linear in the derivatives of the proton and neutron densities, the associated mass number and isospin dependence is very moderate in heavy nuclei. On the other hand, the second term in Eq. (4) depends on the spin density J_q which has a more peculiar behavior. J_q gives essentially no contribution in the spin-saturated cases, but it increases linearly with the number of particles if only one of the spin-orbit partners is filled. The sign of the J_q will change depending upon the quantum numbers of the orbitals which are progressively filled: that is, the orbital with $j_> = l + 1/2$ gives a positive contribution to J_q while the orbital with $j_< = l - 1/2$ gives a negative contribution to J_q. This must be kept in mind to understand the results which are discussed below.

According to Ref. [5], the optimal parameters α_T and β_T should be found in a triangle in the two dimensional (α_T, β_T) plane, lying in the quadrant of negative α_T and positive

β_T. At that time, the force SIII was used. As already mentioned, we wish to use here the Lyon forces which have been fitted using a more complete protocol (including the neutron matter equation of state) and have some better features like a more realistic value of the incompressibilty K_∞. Therefore, we have refitted the values of (α_T, β_T) using the recent experimental data [10] for the single-particle states in the N=82 isotones and the Z=50 isotopes. We have not tried to refit all the Skyrme parameters after including the tensor terms. This can be left for future work. However, we have checked that the binding energies and the r.m.s. charge radii of ^{132}Sn (^{208}Pb) change, respectively, by +0.65% and -0.17% (+0.46% and -0.11%) when we include the tensor force. The parameters we have chosen are α_T = -170 MeV·fm^5 and β_T = 100 MeV·fm^5. We should mention that for the force SLy5, α_C = 80.2 MeV·fm^5 and β_C = -48.9 MeV·fm^5. The fact that we need significantly larger values of (α_T, β_T) as compared to Ref. [5] can be adscribed to the fact that the effect of the central exchange terms, with (α_C, β_C) having opposite sign as the (α_T, β_T) required by our fit, must be counterbalanced.

In Fig. 1, the energy differences of the proton single-particle states, $\varepsilon(h_{11/2}) - \varepsilon(g_{7/2})$, along the Z=50 isotopes are shown as a function of the neutron excess N-Z. The original SLy5 interaction fails to reproduce the experimental trend both qualitatively and quantitatively. Firstly, the energy differences obtained within HF-BCS are much larger than the empirical data. Secondly, starting from the double-magic ^{132}Sn isotope, the experimental data markedly decrease as the neutron excess decreases and reach about 0.5 MeV at the minimum value in ^{112}Sn. On the other hand, using the HF-BCS approach with SLy5 the result is qualitatively the opposite: the energy differences slightly increase as the neutron excess decreases, and there is a maximum around ^{120}Sn. We have studied also several other Skyrme parameter sets and found almost the same trends as that of SLy5.

In the results displayed in Fig. 1, we can see a substantial improvement due to the introduction of the tensor interaction with (α_T, β_T)=(-170,100) MeV·fm^5. This choice gives a very nice agreement with the experimental data in the range 20 $\leq$ (N-Z) $\leq$ 32, both quantitatively and qualitatively. The HF+tensor results can be qualitatively understood by simple arguments, looking at Eq. (4). In the Z=50 core, only the proton $g_{9/2}$ orbital dominates the proton spin density J_p (cf. Eq. (2)); consequently, with a negative value of α_T, the spin-orbit potential (4) is enlarged in absolute value (notice that W_0 is positive and the radial derivatives of the densities are negative), the values of the proton spin-orbit splittings are increased, and the energy difference $\varepsilon(h_{11/2}) - \varepsilon(g_{7/2})$ is reduced with respect to HF-BCS without tensor. This reduction is seen better around N-Z=20: in fact, ^{120}Sn is, to a good extent, spin-saturated as far as the neutrons are concerned so that one gets no contribution from J_n. It should be noticed that the term in α does not give any isospin dependence to the spin-orbit potential for a fixed proton number, but only the term in β can be responsible for the isospin dependence. In a pure HF description, from N-Z=6 to 14, the $g_{7/2}$ neutron orbit is gradually filled and J_n is reduced. Then, the positive value of β_T enlarges in absolute value the spin-orbit potential and increases the spin-orbit splitting, so that the energy difference $\varepsilon(h_{11/2}) - \varepsilon(g_{7/2})$ becomes smaller. Because of pairing, this decrease is not so pronounced in the results of Fig. 1. Moreover, from N-Z=14 to 20, the $s_{1/2}$ and $d_{3/2}$ neutron orbits are occupied and in this region the spin density is not so much changed since the $s_{1/2}$ orbital does not provide any contribution. Instead, for N-Z=20 to 32, the $h_{11/2}$ orbital is gradually filled. This gives a positive contribution to the spin-orbit potential (4) and the the spin-orbit splitting becomes smaller. $\varepsilon(h_{11/2}) - \varepsilon(g_{7/2})$ consequently increases, and this effect is well pronounced in our theoretical results. The magnitude of

β determines the slope of the isospin dependence, so that a larger β would give a steeper slope.

In Fig. 2, the energy difference $\varepsilon(i_{13/2})-\varepsilon(h_{9/2})$ for neutrons ouside the closed N=82 core is plotted as a function of the neutron excess. The notation is the same of the previous figure. Essentially, the same arguments already made in the previous paragraph can be applied in order to understand the results; simply, we should remind that the proton number is increasing from the right (where the last nucleus displayed is ^{132}Sn) to the left (where the first isotope plotted is ^{150}Er). The $1g_{7/2}$ and $2d_{5/2}$ orbitals are rather close in energy, above the last occupied proton state $1g_{9/2}$ of the Z=50 core, and their occupations are affected by the pairing correlations introduced by the BCS approximation. These two proton orbitals have opposite effect on the spin orbit potential (4). Because of its larger value of j, the $1g_{7/2}$ orbital turns out to play a more important role on the spin-orbit potential, when the tensor interaction is included, in the nuclei with N-Z decreasing from 32 to 24. Accordingly, with positive β_T the neutron spin-orbit potential is enlarged in absolute value: the spin-orbit splitting is made larger for these isotones, so that the $i_{13/2}$ orbital is pushed down and the $h_{9/2}$ is pushed up. These changes make the energy gap $\varepsilon(i_{13/2}) - \varepsilon(h_{9/2})$ smaller for the nuclei from N-Z=32 (^{132}Sn) to N-Z=24 (^{140}Ce). Then, the occupation of the $2d_{5/2}$ orbital reverses the trend around N-Z=22 (^{142}Nd). The theoretical trend remains the same until N-Z=14, since the effect of the $2d_{3/2}$ occupation is counterbalanced by the occupation of the $1h_{11/2}$ which is not much higher and enters the active BCS space.

The role of the tensor interaction due to the β_T term is expected from the discussion made by J.M. Blatt and V.F. Weisskopf [11] for the deuteron. In Ref. [12] the same argument was also presented. The role of α_T has not yet been examined in a quantitative way within the mean field calculations, as this term comes from the triplet-odd tensor interaction. The assessment of its role is new, since the triplet-odd tensor interaction was not included in the analysis of Refs. [11, 12]. Recently, Brown *et al.* [13] studied the tensor interactions in ^{132}Sn and ^{114}Sn, based on the parameter set Skx. They considered both positive and negative values of α_T in the HF calculations and they concluded that $\alpha_T < 0$ gives a better agreement with the experimental data. This result is consistent with the present systematic study of the single-particle states in the Z=50 isotopes and N=82 isotones, performed within the HF+BCS model.

The effect of the tensor interactions can be tested on other single-particle states which are empirically known. In this work, we have also considered the relative position of the $2d_{3/2}$ and $1h_{11/2}$ neutron states in ^{132}Sn and ^{100}Sn. In the former case (^{132}Sn), experimentally the two states are the last occupied, with the $2d_{3/2}$ being less bound than $1h_{11/2}$ by about 240 keV (see Fig. 8 of [14]). Theoretically, all the mean field calculations with Skyrme or Gogny forces, as well as the relativistic mean field (RMF) ones, result with the opposite ordering (see Fig. 7 of [15]). In particular, with the SLy5 force employed here, the $1h_{11/2}$ orbital is less bound by 1.76 MeV. The contribution of the added tensor force reduces this value to 0.67 MeV. It has to be noted that the the right position of the $2d_{3/2}$ level may be rather important for the proper description of the low-lying dipole strength in ^{132}Sn. In fact, the results obtained using a Skyrme force in Ref. [16] show that this strength has basically single-particle character; but even in the calculation of Ref. [17], in which the low-lying dipole strength turns out to present a certain degree of collectivity, the energy position of the levels we have mentioned is relevant since the configurations involving the $2d_{3/2}$ hole contribute to about 50% of the low-lying collective state. In the nucleus ^{100}Sn, experimentally the $2d_{3/2}$ level is more bound by 0.9 MeV (see Fig. 7 of [14]). In our HF calculation with the SLy5

force, the two levels have the right order but their energy difference is 2.13 MeV. It is quite satisfactory that this difference becomes 1.33 MeV after including the tensor interactions.

We have already mentioned that total binding energies and charge radii of ^{132}Sn and ^{208}Pb are not extremely sensitive to the tensor interactions. We have also checked in our work the effect of the tensor terms on the isotope shift of the Pb isotopes. Actually, this effect is small (and does not even have the correct sign to reproduce experiment). Thus, the tensor interactions is unable to produce the well-known empirical kink in the trend of the charge radii beyond ^{208}Pb, which instead results from the introduction of generalized spin-orbit functionals [18].

Single-particle energies, and other ground-state properties, are not the only observables which are affected by the inclusion of tensor interactions. There exist excited states which reflect very much the behavior of the spin-orbit splittings. One of them is the well-known Gamow-Teller resonance (GTR). We have made a simple estimate of the effect of the tensor interactions on the GTR centroid by using the sum rules. In charge-exchange RPA calculations, the following sum rules are satisfied [19],

$$\begin{aligned} m_-(0) - m_+(0) &= \langle 0|[F^\dagger, F]|0\rangle, \\ m_-(1) + m_+(1) &= \langle 0|[F^\dagger, [H, F]]|0\rangle. \end{aligned} \tag{8}$$

In the above expressions, $m_\pm(k)$ denotes the k-th moment of the strength in the $\Delta T_z = \pm 1$ channel: in particular, we are considering the non energy-weighted sum rule $m(0)$ and the energy-weighted sum rule $m(1)$. The associated operators F and $F^\dagger$ act, respectively, in the $\Delta T_z = -1$ and $\Delta T_z = +1$ channels. In the Gamow-Teller case, they read

$$\begin{aligned} F &= \sum_i \vec{\sigma}(i) t_-(i), \\ F^\dagger &= \sum_i \vec{\sigma}(i) t_+(i). \end{aligned} \tag{9}$$

Moreover, in Eq. (8), H is the total Skyrme Hamiltonian and $|0\rangle$ is the HF ground state. In nuclei with neutron excess, the contributions associated with the $\Delta T_z = +1$ channel are negligible and we can approximate the GT centroid as

$$E_{GT} = \frac{m_-(1)}{m_-(0)} \sim \frac{\langle 0|[F^\dagger, [H, F]]|0\rangle}{\langle 0|[F^\dagger, F]|0\rangle}. \tag{10}$$

The contribution from the tensor interaction to the GT centroid is obtained by replacing the total Hamiltonian H in the previous formula, with the two-body force of Eq. (1). The calculation of the ground-state expectation value of the double commutator $[F^\dagger, [v_T, F]]$ has been worked out and it gives the contribution of the tensor force to the GT centroid,

$$\Delta E_{GT} = \frac{4\pi}{9(N-Z)} \int dr r^2 [\frac{24}{5}(\beta - 5\alpha) J_p J_n - 12\alpha (J_p^2 + J_n^2)]. \tag{11}$$

We have evaluated this latter expression, for the Sn isotopes having N-Z larger than 20, by using our optimal (α_T, β_T) values of (-170, 100). The results are reported in Table I. The numbers are not small, but this should not be surprising since the shifts of the single-particle states displayed in the Figures can also be of the order of 1-2 MeV. In fact, the positive energy shift can be expected in ^{208}Pb as well and can be understood as follows.

The spin-orbit densities (2) receive contribution only from the $i_{13/2}$ orbital (in the case of neutrons) and from the $h_{11/2}$ orbital (in the case of protons). From Eq. (4), one sees that, since α_T is negative and $|\alpha_T| > |\beta_T|$, the net effect is an increase of the spin-orbit splitting. Consequently, the excitation energy of the dominant unperturbed Gamow-Teller configuration, that is, $\nu i_{13/2} \rightarrow \pi i_{11/2}$, is shifted upwards by the tensor correlations. With similar arguments we can understand the numbers reported in Table I, as we did for the values plotted in the previous Figures. Actually, we should remind that the analysis in terms of the sum rules is not able to tell whether the peak energy is affected as much as the centroid $m(1)/m(0)$ since the main peak does not exhaust, as a rule, the whole strength.

Accurate QRPA calculations of the Gamow-Teller and spin-dipole resonances are reported in Ref. [20]. The behavior of different Skyrme parameter sets, without the tensor contribution, is critically discussed. In fact, no RPA or QRPA calculations including the two-body tensor force are presently available, for any kind of vibrational mode; accordingly, results obtained without the tensor interactions should be still kept as reference until a global refit of the Skyrme plus tensor parameters is carefully accomplished. The tensor force is not only expected to produce effect on the Gamow-Teller states. Other vibrational states (like the low-lying 2^+ which in many systems, once more, reflects the spin-orbit splitting [21]) will be certainly affected.

A further question for future work is the role of correlations beyond mean field. As discussed at length in Ref. [22], the coupling of single-particle states to vibrational states has the net effect of increasing the level density around the Fermi surface by about 30%, by shifting occupied and unoccupied states in opposite directions. Smaller effects are expected for the energy differences we are considering here since these differences involve pairs of states which are either occupied or unoccupied. The net shift may be of the order of few hundreds of keV as estimated from ^{132}Sn [23].

In conclusion, the present work has shed light on the necessity to include the tensor component in the Skyrme framework. The first attempts in this direction were focusing on the effect of the tensor force in magic nuclei but, as we have stressed, if the nuclei are spin-saturated the spin-orbit splittings are not affected at all by the tensor force. The experimental mesurement of the isospin dependence of single-particle energies has opened the possibility to fit the parameters of the zero-range effective tensor force we are employing. Our results show that the introduction of the tensor force can fairly well explain the isospin dependence of energy differences between single-particle proton states outside the Z=50 core, and neutron states outside the N=82 core. We have not attempted to refit a Skyrme force by including the tensor contribution, but we have discussed, by using the case of the Gamow-Teller centroids, that excited state properties will also be affected by the tensor. An ambitious refitting program of Skyrme forces should therefore be undertaken and deformed systems should be considered as well [24]. This is left as a future prospect, together with the role of particle-vibration coupling in this context.

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TABLE I: The effect of the tensor force on the GT centroid, evaluated by means of Eq. (11) using the SLy5 parameter set and the same parameters of the tensor force which have been fitted on the experimental results for the single-particle states, namely (α_T, β_T)=(-170,100) MeV·fm^5. See the text for a discussion of these results.

Nucleus	ΔE_{GT} [MeV]
^{120}Sn	1.49
^{122}Sn	1.55
^{124}Sn	1.74
^{126}Sn	1.99
^{128}Sn	2.21
^{130}Sn	2.48
^{132}Sn	2.64

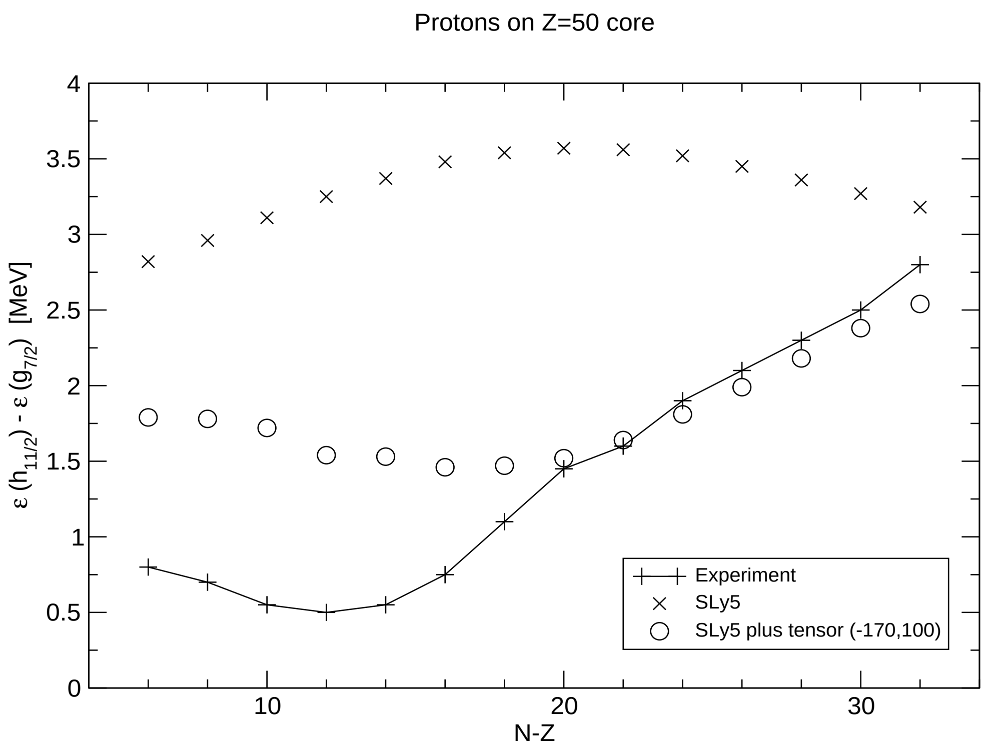

FIG. 1: Energy differences between the 1h$_{11/2}$ and 1g$_{7/2}$ single-proton states along the Z=50 isotopes. The calculations are performed without (crosses) and with (circles) the tensor term in the spin-orbit potential (4), on top of SLy5 (which includes the central exchange, or J^2, terms). The experimental data are taken from ref. [10]. See the text for details.

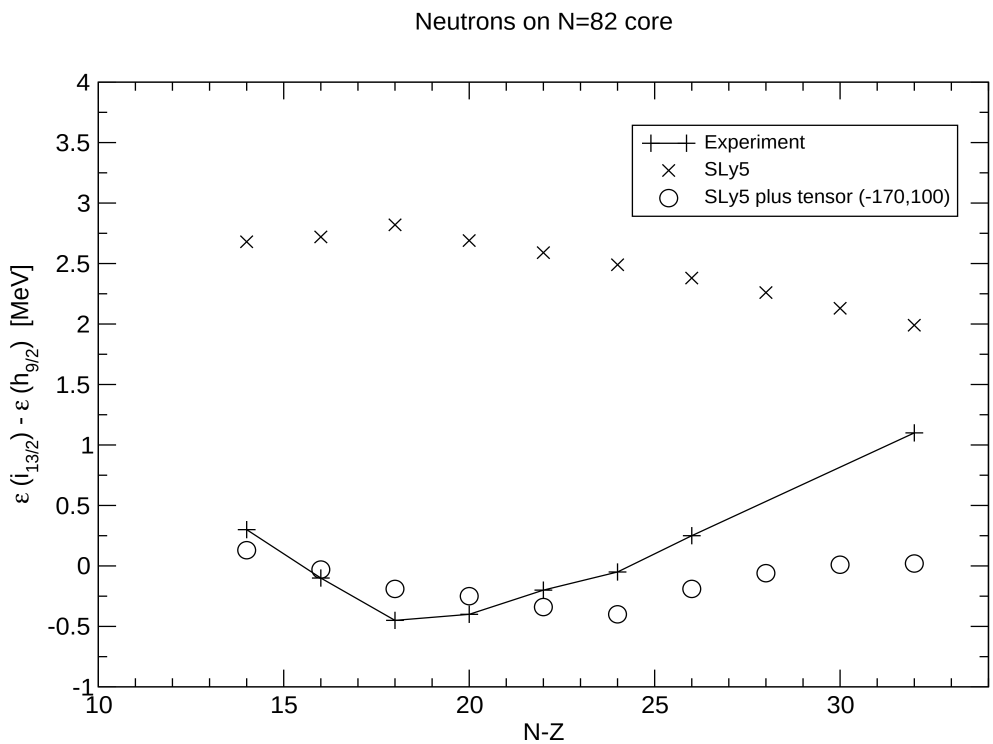

FIG. 2: Energy differences between the $1i_{13/2}$ and $1h_{9/2}$ single-neutron states along the N=82 isotones. The calculations are performed without (crosses) and with (circles) the tensor term in the spin-orbit potential (4), on top of SLy5 (which includes the central exchange, or J^2, terms). The experimental data are taken from ref. [10]. See the text for details.